

=> d his

(FILE 'HOME' ENTERED AT 11:08:17 ON 20 APR 2004)

FILE 'REGISTRY' ENTERED AT 11:09:12 ON 20 APR 2004

L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 24 S L1 SSS FULL  
L4 0 S L2 SSS  
L5 3 S L2 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:11:43 ON 20 APR 2004

L6 11 S L3  
L7 2 S L3 AND L5  
L8 7 S L3/PREP  
L9 2 S L8 AND L5  
L10 2 S L7 OR L9

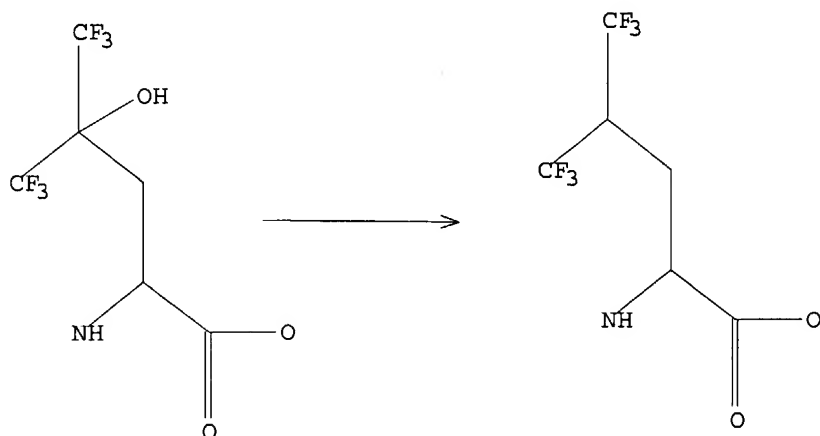
FILE 'CASREACT' ENTERED AT 11:17:16 ON 20 APR 2004

L11 STRUCTURE UPLOADED  
L12 0 S L11

=> d l11

L11 HAS NO ANSWERS

L11 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l11

SAMPLE SEARCH INITIATED 11:18:24 FILE 'CASREACT'

SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS

100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L13 0 SEA SSS SAM L11 ( 0 REACTIONS)

=>

=> d his

(FILE 'HOME' ENTERED AT 11:08:17 ON 20 APR 2004)

FILE 'REGISTRY' ENTERED AT 11:09:12 ON 20 APR 2004

L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 24 S L1 SSS FULL  
L4 0 S L2 SSS  
L5 3 S L2 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:11:43 ON 20 APR 2004

L6 11 S L3  
L7 2 S L3 AND L5  
L8 7 S L3/PREP  
L9 2 S L8 AND L5  
L10 2 S L7 OR L9

FILE 'CASREACT' ENTERED AT 11:17:16 ON 20 APR 2004

L11 STRUCTURE UPLOADED  
L12 0 S L11  
L13 0 S L11

FILE 'CAPLUS' ENTERED AT 11:20:56 ON 20 APR 2004

FILE 'REGISTRY' ENTERED AT 11:38:23 ON 20 APR 2004

L14 STRUCTURE UPLOADED  
L15 2 S L14

FILE 'CAPLUS' ENTERED AT 11:38:42 ON 20 APR 2004

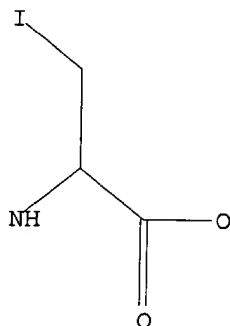
L16 3 S L15  
L17 0 S L16 AND L7  
L18 0 S L16 AND L6  
L19 0 S L5 AND L15

=> d l15

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

=> d l14

L14 HAS NO ANSWERS  
L14 STR



Structure attributes must be viewed using STN Express query preparation.

=>

=> d his

(FILE 'HOME' ENTERED AT 11:08:17 ON 20 APR 2004)

FILE 'REGISTRY' ENTERED AT 11:09:12 ON 20 APR 2004

L1               STRUCTURE UPLOADED  
L2               STRUCTURE UPLOADED  
L3               24 S L1 SSS FULL  
L4               0 S L2 SSS  
L5               3 S L2 SSS FULL

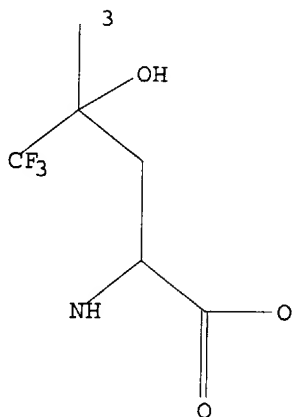
FILE 'CAPLUS' ENTERED AT 11:11:43 ON 20 APR 2004

L6               11 S L3  
L7               2 S L3 AND L5  
L8               7 S L3/PREP  
L9               2 S L8 AND L5  
L10              2 S L7 OR L9

=> d 12

L2 HAS NO ANSWERS

L2               STR



Structure attributes must be viewed using STN Express query preparation.

=> d 12 d bib abs hitstr 1-2

L2 HAS NO ANSWERS

'D BIB ABS HITSTR ' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ----- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ----- Structure Image.

SAT ----- Structure ATtributes and map table if it contains data.

SCT ----- Structure Connection Table and map table if it contains data.

SDA ----- All Structure Data (image, attributes, connection table and map table if it contains data).

NOS ----- NO Structure data.

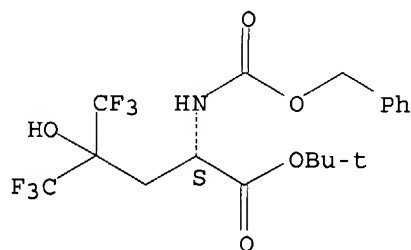
ENTER STRUCTURE FORMAT (SIM), NOS:end

=> d 110 bib abs hitstr 1-2

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:816776 CAPLUS  
DN 138:39519

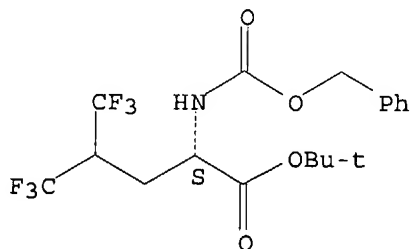
TI A Short and Efficient Synthesis of L-5,5,5,5',5',5'-hexafluoroleucine from N-Cbz-L-Serine  
 AU Anderson, James T.; Toogood, Peter L.; Marsh, E. Neil G.  
 CS Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109, USA  
 SO Organic Letters (2002), 4(24), 4281-4283  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PB American Chemical Society  
 DT Journal  
 LA English  
 OS CASREACT 138:39519  
 AB 5,5,5,5',5',5'-Hexafluoroleucine, H<sub>2</sub>NCH(CO<sub>2</sub>H)CH<sub>2</sub>CH(CF<sub>3</sub>)<sub>2</sub>, a fluorous analog of leucine, is prepared from Cbz-L-Ser-OH by a short and efficient synthesis in 50% overall yield, 99% enantiomeric excess, and in multigram quantities. Key steps are addition of a serine-derived organozincate to hexafluoroacetone to construct the hexafluoroleucine side chain, followed by radical-mediated deoxygenation of the resulting tertiary alc.  
 IT **478548-20-8P 478548-21-9P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP** (**Preparation**); RACT (Reactant or reagent)  
 (preparation of hexafluoroleucine from Cbz-Ser with the addition of hexafluoroacetone to serine-zinc adduct followed by radical-mediated deoxygenation as key steps)  
 RN 478548-20-8 CAPLUS  
 CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-4-hydroxy-N-[(phenylmethoxy)carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



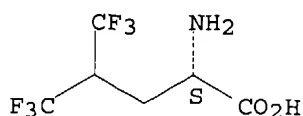
RN 478548-21-9 CAPLUS  
 CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(phenylmethoxy)carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



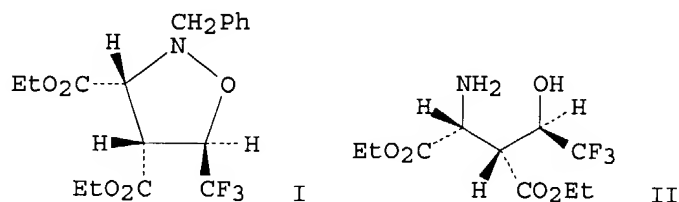
IT **149560-64-5P**  
 RL: SPN (Synthetic preparation); **PREP** (**Preparation**)  
 (preparation of hexafluoroleucine from Cbz-Ser with the addition of hexafluoroacetone to serine-zinc adduct followed by radical-mediated deoxygenation as key steps)  
 RN 149560-64-5 CAPLUS  
 CN L-Leucine, 5,5,5,5',5',5'-hexafluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1993:80452 CAPLUS  
DN 118:80452  
TI A cycloadditive route to trifluoromethyl-substituted amino alcohols  
AU Bravo, Pierfrancesco; Bruche, Luca; Fronza, Giovanni; Zecchi, Gaetano  
CS Cent. Stud. Sostanze Org. Nat., CNR, Milan, I-20133, Italy  
SO Tetrahedron (1992), 48(44), 9775-88  
CODEN: TETRAB; ISSN: 0040-4020  
DT Journal  
LA English  
GI

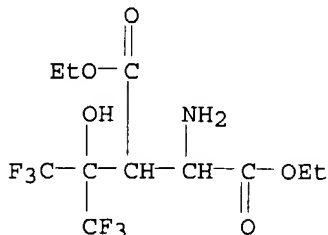


AB A synthetic approach to the title compds. is described, involving the 1,3-dipolar cycloaddn. of nitrones to trifluoromethyl-substituted alkene derivs. followed by reductive ring opening of the so obtained isoxazolidines. Thus, cycloaddn. of EtO2CCH:N+(CH2Ph)O- to (F3C)CH:CHCO2Et gave isoxazolidine I which was hydrogenated to amino alc. II.

IT 145653-41-4P 145653-42-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

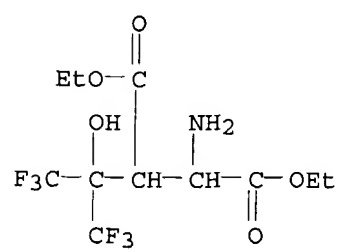
RN 145653-41-4 CAPLUS

CN Aspartic acid, 3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]-, diethyl ester, erythro- (9CI) (CA INDEX NAME)



RN 145653-42-5 CAPLUS

CN Aspartic acid, 3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]-, diethyl ester, threo- (9CI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 11:08:17 ON 20 APR 2004)

FILE 'REGISTRY' ENTERED AT 11:09:12 ON 20 APR 2004

L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 24 S L1 SSS FULL  
L4 0 S L2 SSS  
L5 3 S L2 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:11:43 ON 20 APR 2004

L6 11 S L3  
L7 2 S L3 AND L5  
L8 7 S L3/PREP  
L9 2 S L8 AND L5  
L10 2 S L7 OR L9

FILE 'CASREACT' ENTERED AT 11:17:16 ON 20 APR 2004

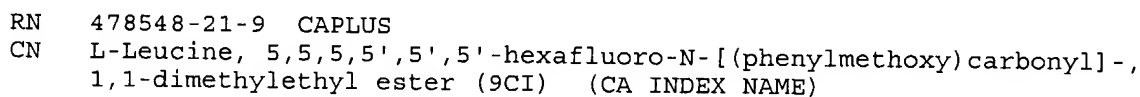
L11 STRUCTURE UPLOADED  
L12 0 S L11  
L13 0 S L11

FILE 'CAPLUS' ENTERED AT 11:20:56 ON 20 APR 2004

=> d 18 bib abs hitstr 1-7

L8 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:816776 CAPLUS  
DN 138:39519  
TI A Short and Efficient Synthesis of L-5,5,5,5',5',5'-hexafluoroleucine from  
N-Cbz-L-Serine  
AU Anderson, James T.; Toogood, Peter L.; Marsh, E. Neil G.  
CS Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109, USA  
SO Organic Letters (2002), 4(24), 4281-4283  
CODEN: ORLEF7; ISSN: 1523-7060  
PB American Chemical Society  
DT Journal  
LA English  
OS CASREACT 138:39519  
AB 5,5,5,5',5',5'-Hexafluoroleucine, H<sub>2</sub>NCH(CO<sub>2</sub>H)CH<sub>2</sub>CH(CF<sub>3</sub>)<sub>2</sub>, a fluorous  
analog of leucine, is prepared from Cbz-L-Ser-OH by a short and efficient  
synthesis in 50% overall yield, 99% enantiomeric excess, and in multigram  
quantities. Key steps are addition of a serine-derived organozincate to  
hexafluoroacetone to construct the hexafluoroleucine side chain, followed  
by radical-mediated deoxygenation of the resulting tertiary alc.  
IT 478548-20-8P 478548-21-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation of hexafluoroleucine from Cbz-Ser with the addition of  
hexafluoroacetone to serine-zinc adduct followed by radical-mediated  
deoxygenation as key steps)  
RN 478548-20-8 CAPLUS  
CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-4-hydroxy-N-[(phenylmethoxy)carbonyl]-  
, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CC(C)(C)OC(=O)C1SC(CF)(C(F)F)NC1C(=O)OCC2=CC=CC=C2

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
(preparation of hexafluoroleucine from Cbz-Ser with the addition of  
hexafluoroacetone to serine-zinc adduct followed by radical-mediated  
deoxygenation as key steps)

CN L-Leucine, 5,5,5,5',5',5'-hexafluoro- (9CI) (CA INDEX NAME)

FC(F)(F)C(C(F)(F)F)C(S)C(=O)O

L8 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:676148 CAPLUS  
DN 137:201607  
TI Synthesis of non-racemic hexafluoroleucine and its incorporation into  
peptides  
IN Fichera, Alfio; Bilgicer, Zihni B.; Kumar, Krishna; Xing, Xuechao  
PA Trustees of Tufts College, USA  
SO PCT Int. Appl., 89 pp.  
CODEN: PIXXD2

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002068592	A2	20020906	WO 2002-US5386	20020225
	WO 2002068592	A3	20030227		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,



CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,  
UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,  
TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,  
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,  
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2001-271999P P 20010227  
US 2001-348091P P 20011029

OS CASREACT 137:201607; MARPAT 137:201607

AB The invention relates to hexafluoroleucine and congeners for the synthesis of protein cores comprising hexafluoroleucine or congeners. Compds. R2NCH[CH2CH(CF3)2]CO-X-R1 [X = O, S, NR, CR2; R = H, alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl, formyl, acyl, alkoxycarbonyl, aralkoxycarbonyl, alkylaminocarbonyl, or aralkylaminocarbonyl; R1 = H, alkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl; or XR1 = halide] are claimed. The stereochem. configuration at any stereocenter of these compds. may be R, S, (enantiomeric excess .gtorsim. 85%) or RS. A novel, short, and efficient synthesis of (S)-5,5,5,5',5',5'-hexafluoroleucine in > 99% ee was carried out starting from Garner's aldehyde, a protected oxazolidine aldehyde. Certain peptides comprising hexafluoroleucine or congeners generally show higher thermal stability and enhanced resistance to chemical denaturation. Mixed hydrocarbon/fluorocarbon cores self-sort into homogeneous bundles, suggesting new avenues for the design and manipulation of protein-protein interfaces.

IT 201930-89-4P 340714-55-8P

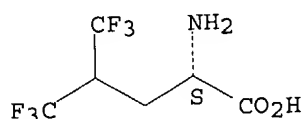
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)

(synthesis of non-racemic hexafluoroleucine and its incorporation into peptides)

RN 201930-89-4 CAPLUS

CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

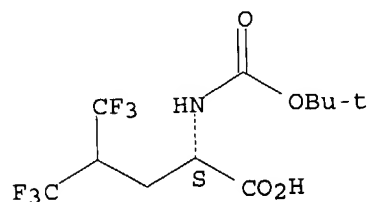


● HCl

RN 340714-55-8 CAPLUS

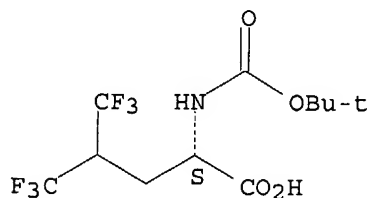
CN L-Leucine, N-[(1,1-dimethylethoxy)carbonyl]-5,5,5,5',5',5'-hexafluoro-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



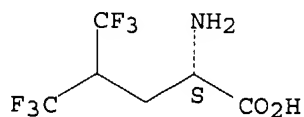
L8 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2001:234530 CAPLUS  
 DN 134:367168  
 TI A Novel Synthesis of Enantiomerically Pure 5,5,5,5',5',5'-  
 Hexafluoroleucine  
 AU Xing, Xuechao; Fichera, Alfio; Kumar, Krishna  
 CS Department of Chemistry, Tufts University, Medford, MA, 02155, USA  
 SO Organic Letters (2001), 3(9), 1285-1286  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PB American Chemical Society  
 DT Journal  
 LA English  
 OS CASREACT 134:367168  
 AB A novel, short, and efficient synthesis of (S)-5,5,5,5',5',5'-  
 hexafluoroleucine (6) in greater than 99% ee was carried out starting from  
 Garner's aldehyde, a protected oxazolidine aldehyde. The enantiomeric  
 excess of the product was calculated from an NMR anal. of a dipeptide formed  
 by reaction with a protected L-serine derivative. Furthermore, a racemic  
 sample of N-acylated hexafluoroleucine was enzymically resolved by  
 treatment with porcine kidney acylase I and was found to have the same  
 optical rotation as a synthetic sample of 6.  
 IT 340714-55-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
 (**Preparation**); RACT (Reactant or reagent)  
 (synthesis of enantiomerically pure hexafluoroleucine)  
 RN 340714-55-8 CAPLUS  
 CN L-Leucine, N-[(1,1-dimethylethoxy)carbonyl]-5,5,5,5',5',5'-hexafluoro-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 201930-89-4P  
 RL: SPN (Synthetic preparation); **PREP** (**Preparation**)  
 (synthesis of enantiomerically pure hexafluoroleucine)  
 RN 201930-89-4 CAPLUS  
 CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-, hydrochloride (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry. Rotation (+).



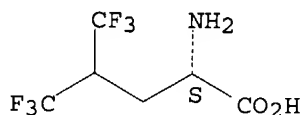
● HCl

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1998:79989 CAPLUS

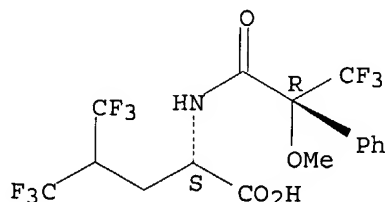
DN 128:128262  
 TI Asymmetric synthesis of (S)-5,5,5,5',5',5'-hexafluoroleucine  
 AU Zhang, Cong; Ludin, Christian; Eberle, Marcel K.; Stoeckli-Evans, Helen; Keese, Reinhart  
 CS Departement Chemie Biochemie, Universitaet Bern, Bern, CH-3012, Switz.  
 SO Helvetica Chimica Acta (1998), 81(1), 174-181  
 CODEN: HCACAV; ISSN: 0018-019X  
 PB Verlag Helvetica Chimica Acta AG  
 DT Journal  
 LA English  
 AB (S)-(CF<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CHNH<sub>2</sub>CO<sub>2</sub>H is prepared starting from (CF<sub>3</sub>)<sub>2</sub>CO and bromopyruvate in 7 steps with 81% ee and 18% overall yield. Key step is the highly enantioselective reduction of the carbonyl group in (S)-(CF<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>COCO<sub>2</sub>Et either by bakers' yeast (91% ee) or by catecholborane utilizing an oxazaborolidine catalyst yielding (R)-(CF<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CHOHCO<sub>2</sub>Et with 99% ee. The absolute configuration was determined by x-ray anal. of the HCl adduct of (2S)-N-[(R)-1-phenylethyl]-(S)-5,5,5,5',5',5'-hexafluoroleucine Et ester.  
 IT 149560-64-5P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)  
 (asym. synthesis and absolute configuration)  
 RN 149560-64-5 CAPLUS  
 CN L-Leucine, 5,5,5,5',5',5'-hexafluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



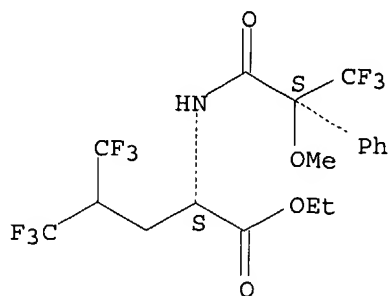
IT 201930-91-8P 201930-93-0P 201930-95-2P  
 201930-97-4P 201930-98-5P 201930-99-6P  
 201931-01-3P 201931-02-4P  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (asym. synthesis and absolute configuration)  
 RN 201930-91-8 CAPLUS  
 CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 201930-93-0 CAPLUS  
 CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]-, ethyl ester (9CI) (CA INDEX NAME)

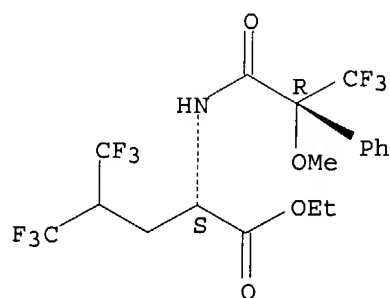
Absolute stereochemistry.



RN 201930-95-2 CAPLUS

CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]-, ethyl ester (9CI) (CA INDEX NAME)

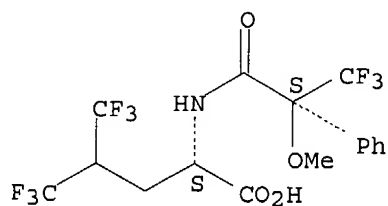
Absolute stereochemistry.



RN 201930-97-4 CAPLUS

CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]- (9CI) (CA INDEX NAME)

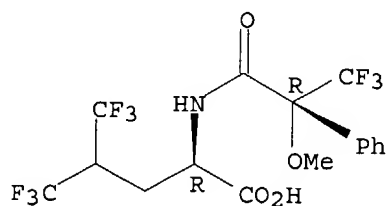
Absolute stereochemistry.



RN 201930-98-5 CAPLUS

CN D-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

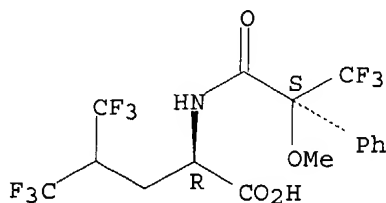


RN 201930-99-6 CAPLUS

CN D-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2S)-3,3,3-trifluoro-2-methoxy-1-

oxo-2-phenylpropyl]- (9CI) (CA INDEX NAME)

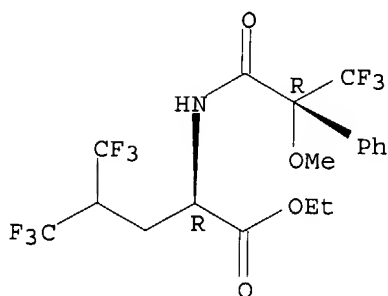
Absolute stereochemistry.



RN 201931-01-3 CAPLUS

CN D-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]-, ethyl ester (9CI) (CA INDEX NAME)

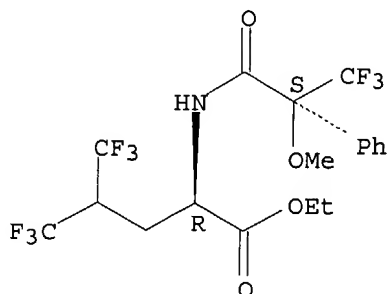
Absolute stereochemistry.



RN 201931-02-4 CAPLUS

CN D-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(2S)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



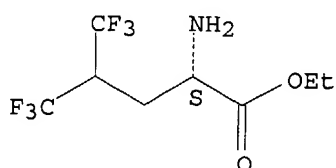
IT 201930-88-3P 201930-89-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(asym. synthesis of fluoroleucine)

RN 201930-88-3 CAPLUS

CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-, ethyl ester, hydrochloride (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

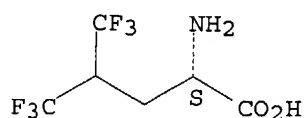


● HCl

RN 201930-89-4 CAPLUS

CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



● HCl

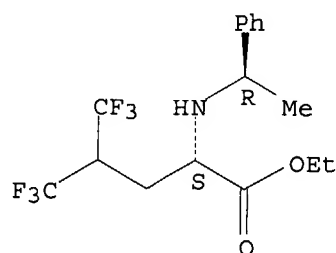
IT 201930-85-0P 201930-87-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(asym. synthesis of fluoroleucine)

RN 201930-85-0 CAPLUS

CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(1R)-1-phenylethyl]-, ethyl ester  
(9CI) (CA INDEX NAME)

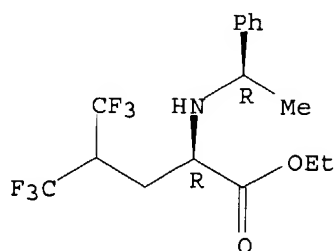
Absolute stereochemistry.



RN 201930-87-2 CAPLUS

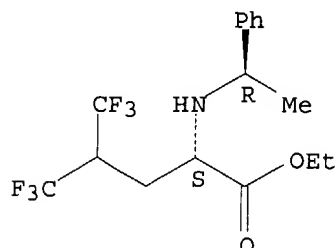
CN D-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(1R)-1-phenylethyl]-, ethyl ester  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



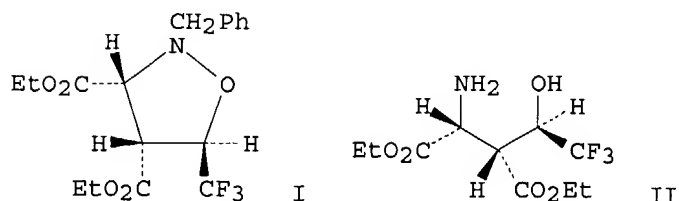
IT 201930-86-1P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);  
**PREP (Preparation)**; RACT (Reactant or reagent)  
 (crystal structure; asym. synthesis of fluoroleucine)  
 RN 201930-86-1 CAPLUS  
 CN L-Leucine, 5,5,5,5',5',5'-hexafluoro-N-[(1R)-1-phenylethyl]-, ethyl ester,  
 hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



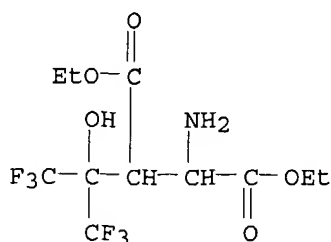
● HCl

L8 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1993:80452 CAPLUS  
 DN 118:80452  
 TI A cycloadditive route to trifluoromethyl-substituted amino alcohols  
 AU Bravo, Pierfrancesco; Bruche, Luca; Fronza, Giovanni; Zecchi, Gaetano  
 CS Cent. Stud. Sostanze Org. Nat., CNR, Milan, I-20133, Italy  
 SO Tetrahedron (1992), 48(44), 9775-88  
 CODEN: TETRAB; ISSN: 0040-4020  
 DT Journal  
 LA English  
 GI

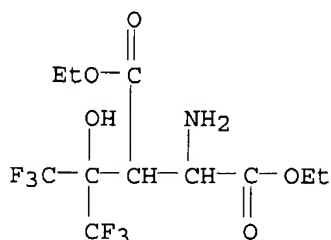


AB A synthetic approach to the title compds. is described, involving the  
 1,3-dipolar cycloaddn. of nitrones to trifluoromethyl-substituted alkene  
 derivs. followed by reductive ring opening of the so obtained  
 isoxazolidines. Thus, cycloaddn. of EtO2CCH:N+(CH2Ph)O- to  
 (F3C)CH:CHCO2Et gave isoxazolidine I which was hydrogenated to amino alc.  
 II.

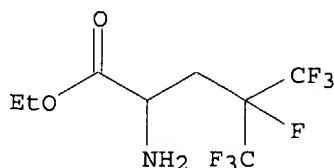
IT 145653-41-4P 145653-42-5P  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (preparation of)  
 RN 145653-41-4 CAPLUS  
 CN Aspartic acid, 3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]-,  
 diethyl ester, erythro- (9CI) (CA INDEX NAME)



RN 145653-42-5 CAPLUS  
 CN Aspartic acid, 3-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]-, diethyl ester, threo- (9CI) (CA INDEX NAME)



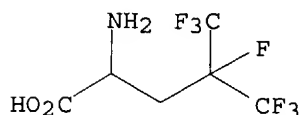
L8 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1977:468600 CAPLUS  
 DN 87:68600  
 TI Synthesis of fluorine-containing DL-alanine derivatives  
 AU Maki, Yasuo; Inukai, Kan  
 CS Ind. Res. Inst., Nagoya, Japan  
 SO Yuki Gosei Kagaku Kyokaishi (1976), 34(10), 722-5  
 CODEN: YGKKAE; ISSN: 0037-9980  
 DT Journal  
 LA Japanese  
 AB Preparation of DL-alanines having a perfluoroalkyl group at the  $\beta$ -position is described. Radical addition of  $\text{CF}_3\text{I}$ ,  $\text{CF}_3\text{CF}_2\text{I}$ ,  $\text{CF}_3(\text{CF}_2)_2\text{I}$ , and  $(\text{CF}_3)_2\text{CFI}$  to  $\text{CH}_2:\text{CHCO}_2\text{Et}$  under UV irradiation gave 23-34%  $\alpha$ -iodo- $\beta$ -(perfluoroalkyl)propionates (I). Reactions of I with  $\text{NaN}_3$  followed by catalytic hydrogenation gave 74-85% of the corresponding F-containing DL-alanine derivs. which on hydrolysis produced the free amino acids.  
 IT 63664-53-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP** (**Preparation**); RACT (Reactant or reagent) (preparation and hydrolysis of)  
 RN 63664-53-9 CAPLUS  
 CN Norvaline, 4,5,5,5-tetrafluoro-4-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



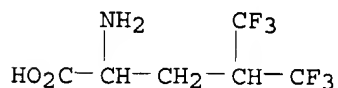
IT 63948-30-1P  
 RL: SPN (Synthetic preparation); **PREP** (**Preparation**) (preparation of)



RN 63948-30-1 CAPLUS  
CN Norvaline, 4,5,5,5-tetrafluoro-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 1968:78588 CAPLUS  
DN 68:78588  
TI Fluorinated analogs of leucine, methionine, and valine  
AU Lazar, Joseph; Sheppard, William A.  
CS Exptl. Sta., du Pont de Nemours, E. I., and Co., Wilmington, DE, USA  
SO Journal of Medicinal Chemistry (1968), 11(1), 138-40  
CODEN: JMCMAR; ISSN: 0022-2623  
DT Journal  
LA English  
AB The fluorinated amino acid analogs trifluorovaline (I), hexafluorovaline (II), and trifluoromethionine (III) were prepared by known methods. Hexafluoroleucine, (CF<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH(NH<sub>2</sub>)CO<sub>2</sub>H (IV), was prepared by treating (CF<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CO<sub>2</sub>H with LiAlH<sub>4</sub>, then with tosyl chloride in pyridine, giving a tosylate which was converted to (CF<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>2</sub>CN by treatment with NaCN in Me<sub>2</sub>SO. This compound was hydrolyzed to the acid, treated with Br and SOCl<sub>2</sub> to give the 2-bromo compound, esterified with EtOH, treated with NaN<sub>3</sub> in EtOH, hydrogenated, hydrolyzed with HCl, and treated with pyridine to give the final product, IV. The pK<sub>a</sub> of these compds. and their amino acid analogs are given. In biol. studies, the growth of Escherichia coli B-14 Leu- was not supported by IV, and I, II, and III did not support the growth of valine and methionine auxotrophs of E. coli K12. The growth of wild type E. coli B and K12 was not inhibited by the F-containing compds., but the latter were not incorporated into the cell protein.  
IT 16063-98-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 16063-98-2 CAPLUS  
CN Valeric acid, 2-amino-5,5,5-trifluoro-4-(trifluoromethyl)- (8CI) (CA INDEX NAME)



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